Package ‘hgm’

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Description The holonomic gradient method (HGM, hgm) gives a way to evaluate normalization constants of unnormalized probability distributions by utilizing holonomic systems of differential or difference equations. The holonomic gradient descent (HGD, hgd) gives a method to find maximal likelihood estimates by utilizing the HGM.
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Description

The holonomic gradient method (HGM, hgm) gives a way to evaluate normalizing constants of unnormalized probability distributions by utilizing holonomic systems of differential or difference equations. The holonomic gradient descent (HGD, hgd) gives a method to find maximal likelihood estimates by utilizing the HGM.

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The HGM and HGD are proposed in the paper below. This method based on the fact that a broad class of normalizing constants of unnormalized probability distributions belongs to the class of holonomic functions, which are solutions of holonomic systems of linear partial differential equations.

Note

This package includes a small subset of the Gnu scientific library codes (http://www.gnu.org/software/gsl/). Then, it might cause a conflict with the package gsl.

References

- http://www.openxm.org

See Also


Examples

```r
## Not run:
example(hgm.ncBingham)
```
The function hgm.ncBingham performs the holonomic gradient method (HGM) for Bingham distributions.

**Description**

The function hgm.ncBingham performs the holonomic gradient method (HGM) for Bingham distributions with the deSolve package in R.

**Usage**

```r
hgm.ncBingham(th, d=rep(1,length(th)+1), logarithm=FALSE,
               ini.method="power", times=NULL, withvol=FALSE, ...)
```

**Arguments**

- **th**
  A (p-1)-dimensional vector which specifies the first (p-1) components of the parameter vector of the Bingham distribution on the (p-1)-dim sphere. The p-th parameter is assumed to be zero.

- **d**
  A p-dimensional vector which specifies the multiplicity of the parameter. The default is all-one vector.

- **logarithm**
  If 'logarithm' is TRUE, then the result is log of the normalizing constant.

- **ini.method**
  The method for computing the initial value. Only "power" is implemented now.

- **times**
  A vector; times in [0,1] at which explicit estimates for G are desired. If time = NULL, the set 0,1 is used, and only the final value is returned.

- **withvol**
  If 'withvol' is TRUE, then the normalizing constant with volume of sphere is returned. Otherwise that without volume is returned. Therefore, if 'withvol' is FALSE and the parameter is zero, then the normalizing constant becomes 1.

- **...**
  Additional parameters for computing initial values. Details are omitted.

**Details**

The function hgm.ncBingham computes the normalizing constant of the Bingham distribution and its derivatives at any specified point. The initial value is computed by the power series expansion.

**Value**

The output is p-dimensional vector G. The first element of G is the normalizing constant and the following (p-1)-elements are partial derivative of the normalizing constant with respect to the first (p-1) components of the parameter 'th'.
The function hgm.ncorthant evaluates the orthant probability, which is the normalization constant of the multivariate normal distribution restricted to the first orthant.

Usage

hgm.ncorthant(x,y,rk_step_size=1e-3)

Arguments

x
   See the description of y.

y
   This function evaluates the orthant probability for the m dimensional multivariate normal distribution whose m by m covariance matrix and the mean vector of size m are x and y respectively.

rk_step_size
   The step size for the Runge-Kutta method to apply the HGM.

Details

The function hgm.ncorthant evaluates the orthant probability, which is the normalization constant of the m-dimensional multivariate normal distribution restricted to the first orthant. It uses the holonomic gradient method (HGM) to evaluate it. The rank of the system of differential equations for the HGM is $2^m$.

Value

The output is the orthant probability.

Author(s)

Tamio Koyama
References


Examples

```
## Example 1. Computing the orthant probability
##
# x <- matrix(c(15,26,23,19,
# 26,47,46,35,
# 23,46,65,38,
# 19,35,38,33), nrow =4)
# y <- c(1,2,3,4)
# hgm.ncorthant(x,y)
```

The function `hgm.ncso3` evaluates the normalization constant for the Fisher distribution on SO(3).

Description

The function `hgm.ncso3` evaluates the normalization constant for the Fisher distribution on SO(3).

Usage

```
hgm.ncso3(a,b,c,t0=0.0,q=1,deg=0,log=0)
```

Arguments

- `a` See the description of `c`.
- `b` See the description of `c`.
- `c` This function evaluates the normalization constant for the parameter Theta=diag(theta_ii) of the Fisher distribution on SO(3). The variables a,b,c stand for the parameters theta_11, theta_22, theta_33 respectively.
- `t0` It is the initial point to evaluate the series. If it is set to 0.0, a default value is used.
- `q` If it is 1, then the program works in a quiet mode.
- `deg` It gives the approximation degree of the power series approximation of the normalization constant near the origin. If it is 0, a default value is used.
- `log` If it is 1, then the function returns the log of the normalizing constant.
Details

The normalization constant $c(\Theta)$ of the Fisher distribution on $SO(3)$ is defined by $\int \exp(\text{trace}(\Theta X))$ where $X$ is the integration variable and runs over $SO(3)$ and $\Theta$ is a $3 \times 3$ matrix parameter. A general HGM algorithm to evaluate the normalization constant is given in the reference below. We use the Corollary 1 and the series expansion in 3.2 for the evaluation.

Value

The output is an array of $c(\Theta)$ and its derivatives with respect to $\Theta_{11}, \Theta_{22}, \Theta_{33}$. It is the vector $C$ of the reference below. When log=1, the output is an array of log of them.

Author(s)

Nobuki Takayama

References


Examples

## Example 1. Computing normalization constant of the Fisher distribution on SO(3)
```
hgm.ncso3(1,2,3)[1]
```

## Example 2. Asteroid data in the paper
```
hgm.ncso3(19.6,0.831,-0.671)[1]
```

---

hgm.p2wishart

The function hgm.p2wishart evaluates the cumulative distribution function of the largest eigenvalues of $W_1^{-1}(W_2)$.

Description

The function hgm.p2wishart evaluates the cumulative distribution function of the largest eigenvalues of $W_1^{-1}(W_2)$ where $W_1$ and $W_2$ are Wishart matrices of size $m \times m$ of the freedom $n_1$ and $n_2$ respectively.

Usage

```
hgm.p2wishart(m,n1,n2,beta,q0,approxdeg,h,dp,q,mode,method,
err,automatic,assigned_series_error,verbose,autoplot)
```
Arguments

\(m\) The dimension of the Wishart matrix.
\(n1\) The degree of freedom of the Wishart distribution \(S1\)
\(n2\) The degree of freedom of the Wishart distribution \(S2\)
\(\beta\) The eigenvalues of inverse(\(S2\))*\(S1\) where \(S1\) and \(S2\) are covariant matrices of \(W1\) and \(W2\) respectively.
\(q0\) The point to evaluate the matrix hypergeometric series. \(q0>0\)
\(\text{approxdeg}\) Zonal polynomials up to the approxdeg are calculated to evaluate values near the origin. A zonal polynomial is determined by a given partition \((k1,...,km)\). We call the sum \(k1+...+km\) the degree.
\(h\) A (small) step size for the Runge-Kutta method. \(h>0\).
\(dp\) Sampling interval of solutions by the Runge-Kutta method. When autoplot=1 or \(dp\) is negative, it is automatically set. If it is 0, no sample is stored.
\(q\) The second value \(y[0]\) of this function is the Prob(\(L1 < q\)) where \(L1\) is the first eigenvalue of the Wishart matrix.
\(\text{mode}\) When mode=c(1,0,0), it returns the evaluation of the matrix hypergeometric series and its derivatives at \(q0\). When mode=c(1,1,(2^m+1)*p), intermediate values of \(F(\text{L1} < x)\) with respect to p-steps of x are also returned. Sampling interval is controlled by \(dp\). When autoplot=1, mode is automatically set.
\(\text{method}\) a-rk4 is the default value. When method="a-rk4", the adaptive Runge-Kutta method is used. Steps are automatically adjusted by err.
\(\text{err}\) When err=c(\(e1,e2\)), \(e1\) is the absolute error and \(e2\) is the relative error. This parameter controls the adaptive Runge-Kutta method. If the output is absurd, you may get a correct answer by setting, e.g., err=c(\(1e-(xy+5), 1e-10\)) or by increasing \(q0\) when initial value at \(q0\) is very small as \(1e-xy\).
\(\text{automatic}\) automatic=1 is the default value. If it is 1, the degree of the series approximation will be increased until \(|(F(i)-F(i-1))/F(i-1)| < \text{assigned\_series\_error}\) where \(F(i)\) is the degree i approximation of the hypergeometric series with matrix argument. Step sizes for the Runge-Kutta method are also set automatically from the assigned\_series\_error if it is 1.
\(\text{assigned\_series\_error}\) assigned\_series\_error=0.00001 is the default value.
\(\text{verbose}\) verbose=0 is the default value. If it is 1, then steps of automatic degree updates and several parameters are output to stdout and stderr.
\(\text{autoplot}\) autoplot=0 is the default value. If it is 1, then this function outputs an input for plot (which is equivalent to setting the 3rd argument of the mode parameter properly). When ans is the output, ans[1,] is c(q,prob at q,...), ans[2,] is c(q0,prob at q0,...), and ans[3,] is c(q+q/100,prob at q/100,...), ... When the adaptive Runge-Kutta method is used, the step size \(h\) may change automatically, which makes the sampling period change, in other words, the sampling points \(q0+q/100, q0+2^2q/100, q0+3^3q/100, ...\) may change. In this case, the output matrix may contain zero rows in the tail or overfull. In case of the overful, use the mode option to get the all result.
Details

It is evaluated by the Koev-Edelman algorithm when x is near the origin and by the HGM when x is far from the origin. We can obtain more accurate result when the variables h is smaller, q0 is relevant value (not very big, not very small), and the approxdeg is more larger. A heuristic method to set parameters q0, h, approxdeg properly is to make x larger and to check if the y[0] approaches to 1.

Value

The output is x, y[0], ..., y[2^m] in the default mode, y[0] is the value of the cumulative distribution function P(L1 < x) at x. y[1],...,y[2^m] are some derivatives. See the reference below.

Note

This function does not work well under the following cases: 1. The beta (the set of eigenvalues) is degenerated or is almost degenerated. 2. The beta is very skew, in other words, there is a big eigenvalue and there is also a small eigenvalue. The error control is done by a heuristic method. The obtained value is not validated automatically.

Author(s)

Nobuki Takayama

References

H.Hashiguchi, N.Takayama, A.Takemura, Distribution of ratio of two Wishart matrices and evaluation of cumulative probability by holonomic gradient method.

Examples

```r
## Example 1.
## hgm.p2wishart(m=3,n1=5,n2=10,beta=c(1,2,4),q=4)
##
## Example 2.
## b<-hgm.p2wishart(m=3,n1=5,n2=10,beta=c(1,2,4),q0=0.3,q=20,approxdeg=20,mode=c(1,1,(8+1)*1000));
## c<-matrix(b,ncol=8+1,byrow=1);
## plot(c)
##
## Example 3.
## c<-hgm.p2wishart(m=3,n1=5,n2=10,beta=c(1,2,4),q0=0.3,q=20,approxdeg=20,autoplot=1);
## plot(c)
```
The function `hgm.pwishart` evaluates the cumulative distribution function of random Wishart matrices.

**Description**

The function `hgm.pwishart` evaluates the cumulative distribution function of random Wishart matrices of size \( m \times m \).

**Usage**

```r
hgm.pwishart(m,n,beta,q0,approxdeg,h,dp,q,mode,method,err,automatic,assigned_series_error,verbose,autoplot)
```

**Arguments**

- **m**
  - The dimension of the Wishart matrix.
- **n**
  - The degree of freedom (a parameter of the Wishart distribution).
- **beta**
  - The eigenvalues of the inverse of the covariance matrix / 2 (a parameter of the Wishart distribution). The beta is equal to \( \text{inverse}(\sigma) / 2 \).
- **q0**
  - The point to evaluate the matrix hypergeometric series. \( q0 > 0 \).
- **approxdeg**
  - Zonal polynomials up to the approxdeg are calculated to evaluate values near the origin. A zonal polynomial is determined by a given partition \((k_1,...,k_m)\). We call the sum \( k_1 + ... + k_m \) the degree.
- **h**
  - A (small) step size for the Runge-Kutta method. \( h > 0 \).
- **dp**
  - Sampling interval of solutions by the Runge-Kutta method. When autoplot=1 or dp is negative, it is automatically set. If it is 0, no sample is stored.
- **q**
  - The second value \( y[0] \) of this function is the \( \text{Prob}(L_1 < q) \) where \( L_1 \) is the first eigenvalue of the Wishart matrix.
- **mode**
  - When mode=c(1,0,0), it returns the evaluation of the matrix hypergeometric series and its derivatives at \( q0 \). When mode=c(1,1,(2^m+1)*p), intermediate values of \( \text{P}(L_1 < x) \) with respect to \( p \)-steps of \( x \) are also returned. Sampling interval is controlled by \( dp \). When autoplot=1, it is automatically set.
- **method**
  - \( \text{a-rk4} \) is the default value. When method=“a-rk4”, the adaptive Runge-Kutta method is used. Steps are automatically adjusted by \( err \).
- **err**
  - When \( err=c(e1,e2) \), \( e1 \) is the absolute error and \( e2 \) is the relative error. This parameter controls the adaptive Runge-Kutta method. If the output is absurd, you may get a correct answer by setting, e.g., \( err=c(1e-(xy+5), 1e-10) \) or by increasing \( q0 \) when initial value at \( q0 \) is very small as \( 1e-xy \).
- **automatic**
  - \( \text{automatic}=1 \) is the default value. If it is 1, the degree of the series approximation will be increased until \( |(F(i)-F(i-1))/F(i-1)| < \text{assigned_series_error} \) where \( F(i) \) is the degree \( i \) approximation of the hypergeometric series with matrix argument. Step sizes for the Runge-Kutta method are also set automatically from the \( \text{assigned_series_error} \) if it is 1.
assigned_series_error

assigned_series_error=0.00001 is the default value.

verbose

verbose=0 is the default value. If it is 1, then steps of automatic degree updates and several parameters are output to stdout and stderr.

autoplot

autoplot=0 is the default value. If it is 1, then this function outputs an input for plot (which is equivalent to setting the 3rd argument of the mode parameter properly). When ans is the output, ans[1,] is c(q,prob at q,...), ans[2,] is c(q0,prob at q0,...), and ans[3,] is c(q0+q/100,prob at q/100,...), ... When the adaptive Runge-Kutta method is used, the step size h may change automatically, which makes the sampling period change, in other words, the sampling points q0+q/100, q0+2*q/100, q0+3*q/100, ... may change. In this case, the output matrix may contain zero rows in the tail or overfull. In case of the overful, use the mode option to get the all result.

Details

It is evaluated by the Koev-Edelman algorithm when x is near the origin and by the HGM when x is far from the origin. We can obtain more accurate result when the variables h is smaller, q0 is relevant value (not very big, not very small), and the approxdeg is more larger. A heuristic method to set parameters q0, h, approxdeg properly is to make x larger and to check if the y[0] approaches to 1.

Value

The output is x, y[0], ..., y[2^m] in the default mode, y[0] is the value of the cumulative distribution function P(L1 < x) at x. y[1],...,y[2^m] are some derivatives. See the reference below.

Note

This function does not work well under the following cases: 1. The beta (the set of eigenvalues) is degenerated or is almost degenerated. 2. The beta is very skew, in other words, there is a big eigenvalue and there is also a small eigenvalue. The error control is done by a heuristic method. The obtained value is not validated automatically.

Author(s)

Nobuki Takayama

References


Examples

```r
## Example 1.

hgm.pwishart(m=3,n=5,beta=c(1,2,3),q=10)
```
### Example 2.

```r
b<-hgm.pwishart(m=4,n=10,beta=c(1,2,3,4),q0=1,q=10,approxdeg=20,mode=c(1,1,(16+1)*100));
c<-matrix(b,ncol=16+1,byrow=1);
#plot(c)
```

### Example 3.

```r
c<-hgm.pwishart(m=4,n=10,beta=c(1,2,3,4),q0=1,q=10,approxdeg=20,autoplot=1);
#plot(c)
```

---

**hgm.Rhgm**

The function `hgm.Rhgm` performs the holonomic gradient method (HGM) for a given Pfaffian system and an initial value vector.

**Description**

The function `hgm.Rhgm` performs the holonomic gradient method (HGM) for a given Pfaffian system and an initial value vector with the deSolve package in R.

**Usage**

```r
hgm.Rhgm(th0, G0, th1, dG.fun, times=NULL, fn.params=NULL)
```

**Arguments**

- `th0`: A d-dimensional vector which is an initial point of the parameter vector $\theta$.
- `G0`: A r-dimensional vector which is the initial value of the vector $G$ of the normalizing constant and its derivatives.
- `th1`: A d-dimensional vector which is the target point of $\theta$.
- `dG.fun`: `dG.fun` is the “right hand sides” of the Pfaffian system. It is a d*r-dimensional array.
- `times`: a vector; times in [0,1] at which explicit estimates for $G$ are desired. If `times = NULL`, the set 0,1 is used, and only the final value is returned.
- `fn.params`: `fn.params`: a list of parameters passed to the function `dG.fun`. If `fn.params = NULL`, no parameter is passed to `dG.fun`.

**Details**

The function `hgm.Rhgm` computes the value of a holonomic function at a given point, using HGM. This is a “Step 3” function (see the reference below), which can be used for an arbitrary input, in the HGM framework. Efficient “Step 3” functions are given for some distributions in this package.

The Pfaffian system assumed is $\frac{d G_j}{d \theta_i} = (dG.fun(\theta, G))_{ij}$.
The inputs of hgm.Rhgm are the initial point \( \mathbf{t}_0 \), initial value \( \mathbf{G}_0 \), final point \( \mathbf{t}_1 \), and Pfaffian system \( \mathbf{dG} \). The output is the final value \( \mathbf{G}_1 \).

If the argument ‘times’ is specified, the function returns a matrix, where the first column denotes time, the following d-vector denotes \( \mathbf{t} \), and the remaining r-vector denotes \( \mathbf{G} \).

**Value**

The output is the value of \( \mathbf{G} \) at \( \mathbf{t}_1 \). The first element of \( \mathbf{G} \) is the normalizing constant.

**Author(s)**

Tomonari Sei

**References**

[http://www.math.kobe-u.ac.jp/OpenXM/Math/hgm/ref-hgm.html](http://www.math.kobe-u.ac.jp/OpenXM/Math/hgm/ref-hgm.html)

**Examples**

```r
# Example 1.
# A demo program; von Mises--Fisher on \( S^{3-1} \)

G.exact = function(th){  # exact value by built-in function
  c( sinh(th[1])/th[1], cosh(th[1])/th[1] - sinh(th[1])/th[1]^2 )
}

dG.fun = function(th, G, fn.params=NULL){  # Pfaffian
  dG = array(0, c(1, 2))
  dG
}

th0 = 0.5
th1 = 15

G0 = G.exact(th0)

G0

G1 = hgm.Rhgm(th0, G0, th1, dG.fun)  # HGM

G1

G1.exact = G.exact(th1)

G1.exact

#          # Example 2.
#          # hgm.Rhgm.demo1()
```

**Example 2.**

hgm.Rhgm.demo1()
The function hgm.Rhgm.demo1 performs a demonstration of the function hgm.Rhgm.

Usage

hgm.Rhgm.demo1()

Details

The function hgm.Rhgm.demo1 evaluates the normalizing constant of the Von-Mises distribution by the HGM.

Value

The returned value is a dataframe. The column exact of the dataframe is the exact value of the normalizing constant. The column byHGM is the value obtained by the HGM. The column start is the initial value for the HGM.

Author(s)

Tomonari Sei

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